It's All In the GAMESS

Chemistry code unravels molecular mysteries

by Saren Johnston

Mark Gordon (pointing) discusses GAMESS and other projects underway in the Scalable Computing Lab with Secretary of Energy Spencer Abraham when the Secretary visited Ames Laboratory's booth at Supercomputing 2002 in Baltimore.

What molecules do and why they do it is largely an enigma, a puzzle of giant proportions. But when all is said and done, it's molecular events that, simply put, make up the days of our lives. So it's not surprising that scientists continue to search for the reasons governing the actions and reactions of these mighty bits of matter.

Among those who are looking for answers to problems relating to molecules is Mark Gordon, Ames Laboratory program director of Applied Mathematics and Computational Sciences and head of Ames Lab's Scalable Computing Lab. Odds are Gordon may be having better luck at the search than others, luck being somewhat of a misnomer as it implies a certain degree of chance, and Gordon has not left this investigation to the game of chance.

No games, just GAMESS

Gordon and his Ames Laboratory coworkers are fostering and expanding a computational chemistry code that provides extensive and detailed information about how things work on the molecular scale.

The General Atomic and Molecular Electronic Structure System, known as GAMESS, includes a hierarchy of quantum chemistry methods that helps solve problems relating to molecules, making possible the design of new fuels and optical materials and the development of coatings that are resistant to extreme environments.

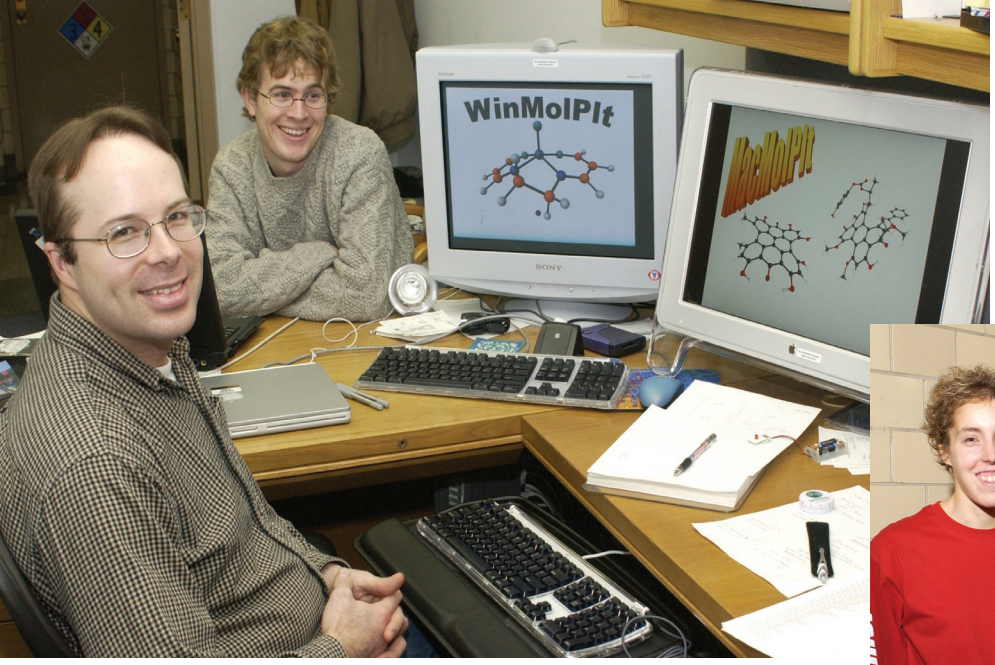
"All of chemistry, which also means all of biology, fundamentally involves molecular processes — that is, the way molecules react or behave," says Gordon, who is also an Iowa State University Distinguished Professor of Chemistry. "Chemistry, biochemistry, biology, materials science, physics — all ultimately can be reduced to what molecules do and why they do it. GAMESS allows you to answer those questions."

Using GAMESS, Gordon, his co-workers and the students in his research group are making major contributions to the design of new rocket fuels for the Air Force. "We're also involved in a Grand Challenge program for the Department of Defense, using GAMESS to help design new optical materials, fuels and wear-resistant coatings," says Gordon. "Some of my former students are now using GAMESS to study biological processes, such as protein behavior."

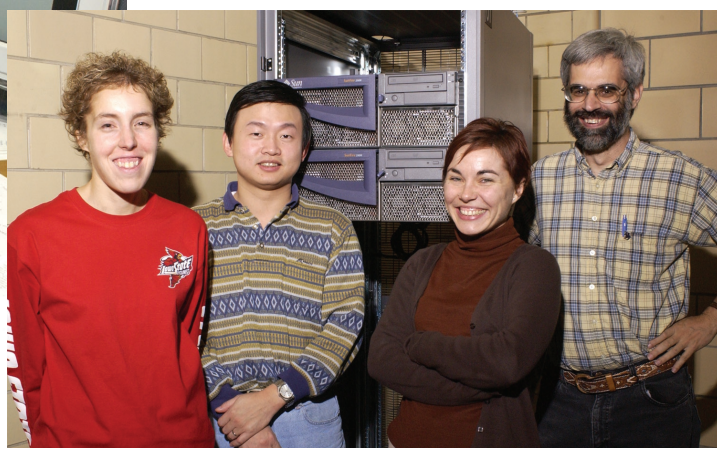
Historically speaking

The history of GAMESS goes back to 1977 when the initial version of the code was assembled, under the direction of Dr. Michael Dupuis, from several existing quantum chemistry computer programs by the staff at the National Resource for Computations in Chemistry. The original project was funded by the National Science Foundation and the Department of Energy from 1977 to 1981. However, the continued development of GAMESS from 1982 to present is directly due to the funding provided by the Air Force Office of Scientific Research; to the nurturing environment provided by Gordon; and to the expertise demonstrated by Gordon, Ames Lab associate Michael Schmidt and many students and postdoctoral fellows in developing new functionalities and parallelizing the code. Making a code operate efficiently in parallel refers to organizing it so that it can take advantage of parallel computers — those with several processors that can work on different parts of a single problem simultaneously. Also, contributions to the GAMESS program from Gordon's many colleagues and from students who have been in his research group have added tremendously to the current robust nature of the code.

"GAMESS is what's called a legacy code," says Gordon. "It existed far before anything of its kind, so some features of GAMESS have been made parallel from the beginning, and some features have been made parallel after the fact. I've always had at least two or three students and postdocs specifically working on how to make GAMESS more parallel," he says. "It's our forte — what we like to do is develop these very sophisticated methods, in many cases with colleagues, and make them parallel and more efficient so we can apply them to bigger molecular systems. It's something we do better than most." A major result of this ongoing effort



Brett Bode (foreground) and Ryan Olson bring the results of complicated GAMESS calculations to life through their respective visualization programs, MacMolPlt and WinMolPlt.



Members of the Gordon group working on GAMESS enhancements are, left to right, Heather Netzloff, Jie Song, Ivana Adamovic and Michael Schmidt. The researchers will make good use of the two Sun systems pictured behind them in developing new GAMESS techniques.

by the Gordon group is that an increasing percentage of the features in GAMESS, especially the most computationally demanding ones, can be done in parallel.

Supplementing the software suite

In addition to excelling at writing parallel code for GAMESS, Gordon and his Ames Lab collaborators, Schmidt and Klaus Ruedenberg, who is also an ISU Distinguished Professor of Chemistry, are particularly adept at creating sophisticated and complex methods for the software suite that address unusual chemical species.

"When you have chemical reactions going on, especially under severe conditions, such as high temperature or high pressure, you encounter chemical species that you would not even call molecules," Gordon explains. "These are things that don't hang around very long, and you may never see them. They're intermediates and may have lifetimes of only picoseconds or femtoseconds, but they may be very important in the overall reaction process. One of our goals is to develop methods to treat these very unusual species, and the more nontraditional the method, the harder it is to make parallel."

An innovative research tool, GAMESS includes a novel graphics visualization program, MacMolPlt, written for Macintosh computers by Ames Lab associate scientist, Brett Bode. Gordon says MacMolPlt eases the task of interpreting the various complicated calculations performed by GAMESS. Ryan Olson, a graduate student in Gordon's group, is developing WinMolPlt, a Windows version of MacMolPlt. "Ryan has half a dozen people around the world testing this program, so now you can visualize the results of GAMESS calculations if you have a Mac or a PC," says Gordon.

A unique feature of GAMESS is the effective fragment potential, or EFP, which was initially developed by Gordon and Jan Jensen, a former graduate student of Gordon's now at the University of Iowa, in collaboration with Dr. Walter Stevens and his group at the National Institute of Standards and Technology. Stevens is now director of the DOE Chemical Sciences Program. Over the past decade, several graduate students and postdoctoral fellows working with Gordon have contributed to the development of the EFP method, including current students Heather Netzloff and Ivana Adamovic and postdoctoral associate Jie Song.

"Sometimes scientists deal with systems in which there are so many atoms and electrons that quantum mechanics can't be done, even at simple levels," says Gordon. The EFP method is based on quantum mechanics, but it's not quantum mechanics — it's a simple but sophisticated model potential that represents most of the quantum mechanics effects at a very reduced computational effort. The EFP method can be combined with actual quantum mechanics in such a way that a quantum mechanical description is required only in that part of a chemical system that is undergoing a chemical change. The remainder of the system is treated with EFPs, so that the entire calculation takes orders of magnitude less computer time than a fully quantum calculation.

"The EFP is a sophisticated model to predict how solvents effect chemical reactions and to predict the behavior of liquids," says Gordon, "and it's working very well.

GAMESS offers an amalgam of choices for quantum mechanical modeling of molecular systems. As such, it proves to be an indispensable tool for today's chemical researchers who have the benefit and availability of increasing computational power to probe the molecular world. Evidence of its capabilities is the fact that GAMESS is used at well over 5,000 sites worldwide, ranging from high schools and research universities in the United States and abroad to government laboratories and the private sector. And best of all, GAMESS is distributed at no cost to users by accessing *www.msg.ameslab.gov* and signing a license agreement. ◆

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